THEORETICAL STUDY OF THE ELECTRON CAPTURE IN PROTON HYDROGEN ATOM SCATTERING

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ABSTRACT

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Coupled state calculations of proton-hydrogen atom scattering have been performed, and the results are reported in this thesis. The excitation matrix elements are evaluated analytically. The initial three-dimensional integrals are first reduced to one-dimentional integrals using a Feynman technique. A Gauss-Lequerre integral method is used to compute this integral. The 1s-3s charge transfer cross sections for proton-hydrogen scattering have been evaluated and compared with available results.

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CHAPTER ONE

INTRODUCTION

The study of charge transfer is important, not only in order to obtain an understanding of the basic mechanism of rearrangement collisions, but also because charge transfer is a process which plays a vital role in the formation of decay of both astrophysical and laboratory plasmas. Charge transfer is also useful in thermonuclear research and atmospheric physics.

Charge transfer reaction in atomic physics is one in which an electron, or several electrons are transferred from one atomic system to another. This was discovered in 1923[1] during the course of experiments in which α-particles were passed through absorbing screens of mica. Numbers of singly charged He^+ ions and also neutral He atoms were observed to emerge from the far side of the screens, and these were attributed to the capture of electrons by the α- particles. The interpretation of Henderson's experiment was confirmed and the measurements extended to electron capture by α-particles from air and hydrogen, by Rutherford [2], Henderson [3] and Jacobson[4]. Charge transfer in the reactions of protons and hydrogen have received a great deal of attention. The first experimental studies of charge transfer and ionization in proton-hydrogen collisions were reported in 1958[5]. Several theoretical methods such as Born series [6-18], distortion approximation [19-20] impulse approximation [21-23], molecular state expansion [24-26] and atomic state expansion [27-36] have been used to evaluate the cross sections of electron exchange.

The first applications of quantum mechanics to charge transfer were perturbation treatments by Oppenheimer [6] and by Brinkman and Kramers [3]. The latter authors were the first to make use of the fact that, at all energies except the very lowest energies, the wavelength associated with the relative motion of the heavy par-

ticle is very small compared with the distance over which interaction takes place, with the consequence that the heavy-particle motion follows a classical Newtonian trajectory; only the electronic motion needs to be treated by quantum mechanics. At low energies the charge transfer cross section is large and a perturbation treatment is not adequate. When the relative velocity of the heavy particles is small, the interaction time is long compared with the characteristic times of electrons in bound state orbits. Under these circumstances the electron to be captured is shared between the two ions during the collision, forming a quasi-molecule. As the ions separate, the probabilities of capture by the projectile or of remaining electrons associated with the target ion are comparable.

When the relative velocity between the nuclei is not small compared to the orbital velocity of the electron, a wave formulation of the method of atomic states has been given by Bates [19]. Most of the detailed calculations for charge transfer in heavy particle collisions are done using the impact parameter method. It assumes that the two nuclei move in a classical straight line trajectory with constant relative velocity. It has been shown that for proton-hydrogen collisions the assumption is valid down to the impact energies of the order of a hundred electron volts. The problem is thus simplified to that of finding the solutions of the time-dependent Schrödinger equation for an electron with appropriate initial conditions. McElroy [20] calculated charge exchange cross sections for $1s-2s$ and $1s-2p$ in proton hydrogen collisions using a distortion approximation. McCarrol [27], Lovell and McElroy[26] did calculations of $1s-1s$ and $1s-2s$ charge transfer using two-center, two-state expansions. Wilets and Gallaher[29] performed couple-channel calculations.

Several methods have been used in calculating charge transfer processes. Toward this end, the reduction of the three-dimensional integrals to one-dimensional

integrals and computing them numerically presents a considerable savings in computer time. Gallaher and Msezane[38] derived one dimensional integrals in which the integrals involved the sum of product of Bessel functions and are complex even for $s-s$ matrix elements. A great deal of experimental and theoretical work has been done on proton-hydrogen charge transfer reactions for $1s/2s/2p_0/2p_1$. A limited number of calculations have been done for $n=3$. Unfortunately, numericaly problems caused some of these results to be quite inaccurate.

In this work, the coupled channel two state approximation method will be used in the calculation of charge transfer cross sections of 1s-3s for collisions between protons and hydrogen atoms.

In Chapter Two we discuss the basic theory of proton-hydrogen collision system. A semiclassical model will be used in our calculation. The nucleus of the target is fixed at the origin of the coordinate system during the collision process. The proton is assumed to follow a straight line trajectory. The trial wave function will be expanded around two centers.

In Chapter Three excitation matrix elements will be calculated for target 1s-1s and projectile 3s-3s. A general expression is obtained from out of the radial part of the integral and this is used for the evaluation.

In Chapter Four charge transfer matrix elements will be evaluated by a one-dimensional integral method. Matrix elements will be used to calculate the charge transfer cross sections in proton-hydrogen scattering. The resultant coupled-channel equations will be solved by using Runge-Kutta method. Charge transfer cross-sections in the energy range of 5-350 keV for $1s-3s$ will be graphed. [B In Chapter Five our results are compared with those of Shakeshaft [33] and Rapp [32]. Comments on our results and suggestions for future extensions are made.

CHAPTER TWO

THEORETICAL APPROACH

Consider a bare nucleus with charge $Z_p e$ incident on a target atom in which the nucleus with charge $Z_t e$ is fixed at the origin of the coordinate system during the collision process. The coordinate system is described in Fig. I. Here $\vec{R}$ and $\vec{r}$ are the position vectors of the projectile (mass M) and target electron (mass m). The total Hamiltonian in the laboratory system is

$$H_t = -\frac{\hbar^2}{2M} \nabla_R^2 - \frac{\hbar^2}{2m} \nabla_r^2 + V_p(|\vec{r} - \vec{R}|) + V_t(\vec{r}) + V_R \quad , \tag{2.1}$$

where V_p, V_t and V_R are the potential energies between projectile nucleus-electron, target nucleus-electron, and nucleus of target and projectile respectively. At a fixed time the total wave function Φ satisfies the wave equation given by

$$H_t \Phi = E \Phi \tag{2.2}$$

The electron will be described by a stationary state wave function $\Psi(\vec{r}, \vec{R})$ satisfying

$$[-\frac{\hbar^2}{2m} \nabla_r^2 + V_p + V_t] \; \Psi \; (\vec{r}, \vec{R}) = \epsilon \; \Psi \; (\vec{r}, \vec{R}) \tag{2.3}$$

The total wave function will be a linear combination of $\Psi(\vec{r}, \vec{R})$.

$$\Phi = \sum_i^N P_i(\vec{R}) \Psi_i(\vec{r}, \vec{R}) \tag{2.4}$$

Substituting eq. (2.4) into eq. (2.2) and using eq.(2.3), we obtain

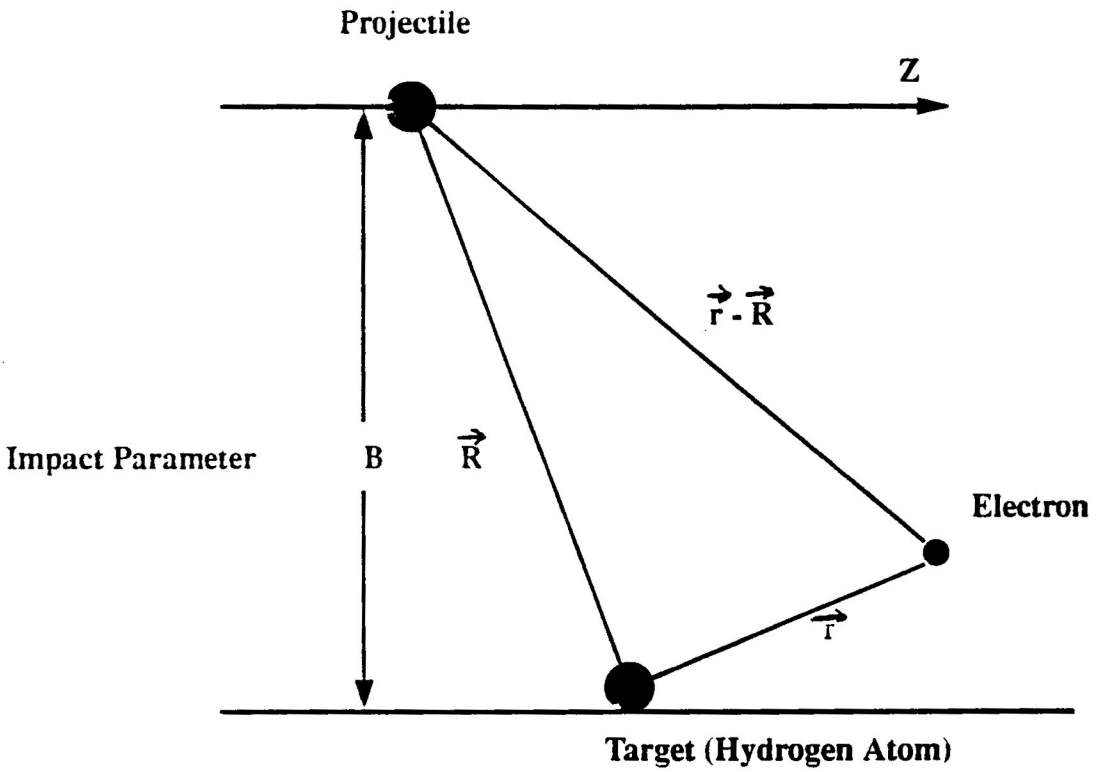

Fig.1. Collision and coordinate system

$$\sum[V_R - \frac{\hbar^2}{2M}\nabla_R^2]P_i\Psi_i = \sum_i(E-\epsilon_i)P_i\Psi_i \tag{2.5}$$

Multiplying by $< \Psi_j|$ in eq. (2.5), we find

$$< \Psi_j \mid \nabla_R^2 \mid P_i\ \Psi_i > = P_i W_{ji} + \delta_{ji}\ \nabla_R^2\ P_i + 2U_{ji}\ \nabla_R\ P_i \tag{2.6}$$

where

$$W_{ji} =< \Psi_j| \nabla_R^2 \mid \Psi_i >$$

and

$$U_{ji} =< \Psi_j| \nabla_R \mid \Psi_i >$$

When the electronic wave function Ψ_i is slowly varying, functions of R, W_{ji} and U_{ji} will be small. Then P_j is the solution of

$$(V_R - \frac{\hbar^2}{2M}\nabla_R^2)P_j = E_j P_j\ , \tag{2.7}$$

where $E_j = E - \epsilon_j$. Eq(2.7) is the required equation of motion for the nuclei. Eqs. (2.3) and (2.7) allow us to separate consideration of the electronic states from consideration of the motion of the nuclei of the atomic system. The description of the atomic process is greatly simplified by the fact that the mass m of the electron is much smaller than the mass M of the nucleus. Therefore, the energy transfer to the electron is a negligible part of the nuclear collision energy. The de Broglie wavelength of the heavy ion is very small compared with atomic dimensions. In practice we may use the classical analysis rather than solve eq. (2.7). The

trajectories of heavy particles are often defined by a classical path which may be distinguished by an impact parameter $\vec{B}$ and a velocity $\vec{v}$. On the contrary, the electronic motion which is associated with the discrete nature of atomic states must be described by quantum mechanics. This reduces the quantum mechanical problem to a semiclassical one. The electronic motion is obtained by solving the time-dependent Schrödinger equation where the time-varying potential arises through $R(t)$

$$(H - i\hbar\frac{\partial}{\partial t})\Psi = 0 \tag{2.8}$$

where

$$H = -\frac{\hbar^2}{2m}\nabla_r^2 - \frac{e^2}{r} - \frac{e^2}{|\vec{r} - \vec{R}|} \tag{2.9}$$

Eq. (2.8) is multiplied through from the left by $\frac{1}{Z_t e^2}$, and the relationships

$$a_B = \frac{\hbar^2}{me^2} \quad , \tag{2.10}$$

$$v_e = \frac{Z_t e^2}{\hbar} \quad , \tag{2.11}$$

$$v = \frac{v_p}{v_o} \quad , \tag{2.12}$$

are noted. Eq. (2.8) may be written as

$$iv\frac{\partial}{\partial z}\Psi = -(\frac{1}{2}\nabla_r^2 - \frac{1}{r} - (\frac{1}{|\vec{r} - \vec{R}|}))\Psi \tag{2.13}$$

In eq. (2.13) $\frac{a_B}{Z_t}$ is used as the unit of length.

For faster collisions where the orbital velocity of the electron is not large compared to the velocity of the projectile, it is common to expand the time-dependent electronic wave function Ψ in terms of atomic eigenstates

$$\Psi(\vec{r},t) = \sum_n a_n(t)\chi_n + \sum_m b_m(t)\phi_m \tag{2.14}$$

In eq. (2.14) χ_n and ϕ_m are atomic eigenstates or pseudostates centered on target or projectile respectively. The usefulness of such an expansion depends on whether the expansion can be truncated to only a few terms. If we are interested only in direct excitation, the electron density concentration near the projectile is small; therefore, the expansion around the projectile can be neglected. Then a single-center expansion (SCE) is suitable and eq. (2.14) reduces to

$$\Psi(\vec{r},t) = \sum_n a_n(t)\chi_n \tag{2.15}$$

The advantage of the SCE is that matrix elements can be expressed as the functions of R only and quickly calculable angular factors e.g. $\frac{Z}{R}, \frac{B}{R}$. Thus the elements need not be recalculated for different impact parameters.

As the collision velocity decreases, the orbiting electron becomes more likely to be pulled to the vicinity of the projectile. The electron will have substantial probability to be in the vicinity of the projectile, especially when $Z_p \sim Z_T$. In this case a two-center expansion is more appropriate. The cross section for electron transfer often peaks near $v \sim v_e$. The electron capture occurs primarily at impact parameters comparable to or greater than the orbital radius of the electron in the initial state. In the two-center expansion (TCE); a translational factor needs to be introduced in the projectile wave function to preserve Galilean invariance. This

factor ensures that the calculation is independent of the choice of the origin. The transformation of an arbitrary wave function χ (defined in the target correlated frame) into the projectile correlated frame and vice versa can be expressed as [39]

$$\phi(\vec{r}\,',t) = S\chi(\vec{r},t), \tag{2.16}$$

$$\chi(\vec{r},t) = S^{+}\phi(\vec{r}\,',t), \tag{2.17}$$

$\vec{r}$ and $\vec{r}\,'$ denote the location of the electron relative to the target and projectile respectively. In the case of a linear motion, S reduces to a Galilean transformation. In our coordinate system, S is

$$S = e^{-i\frac{vZ}{2}}e^{i\vec{v}\cdot\vec{r}} \tag{2.18}$$

Summarizing all these factors the wave function for target 1s and projectile $3s$ states are given by

$$\chi_{1s} = \sqrt{\frac{1}{4\pi}}2e^{-r}e^{-iE_{1s}\frac{z}{v}} \tag{2.19}$$

$$\phi_{3s} = \sqrt{\frac{1}{4\pi}}(\frac{1}{3})^{\frac{3}{2}}[2-\frac{4}{3}|\vec{r}-\vec{R}|+\frac{4}{27}|\vec{r}-\vec{R}|^2]e^{-\frac{|\vec{r}-\vec{R}|}{3}}e^{-iE_{3s}\frac{Z}{v}}e^{-i\frac{v}{2}z}e^{i\vec{v}\cdot\vec{r}} \tag{2.20}$$

The electronic Hamiltonian H may be written as

$$H = H_0 + V \tag{2.21}$$

where H_0 is the unperturbed atomic Hamiltonian, and $V(r,t)$ is a time dependent perturbation which goes to zero as t goes to infinity. The pertubation

$V(r,t)$ of the electronic states will lead to a transition between the initial state i and the final state f with a probability ρ_{ij}. The cross section for transition from initial state i to final state f is then

$$\sigma_{if} = 2\pi \int_0^\infty \rho_{ij} B dB$$

or

$$\sigma_{if} = 2\pi \int_0^\infty |b_{3s}|^2 B dB \tag{2.22}$$

where $\rho_{ij} = |b_{3s}|^2$ = probability.

CHAPTER THREE

EXCITATION MATRIX ELEMENTS

Excitation of an electron is caused by the impact of a fast moving ion or proton on an atom. The process is usually called "direct-excitation". In this work excitation matrix elements are calculated analytically for 1s-1s and 3s-3s. A general integral used to calculate excitation matrix elements is

$$I = \int r^{k_1} e^{-\alpha_1 r} Y_{l_1}^{*m_1}(\vec{r})[-\frac{1}{|\vec{r}-\vec{R}|}]r^{k_2} Y_{l_2}^{m_2}(\vec{r}) e^{-\alpha_2 r} d\vec{r}$$

where $Y_{l,m}(\theta\ ,\phi)$ are spherical Harmonics, (λ_1, λ_2) are $(1s, 1s)$ or $(3s, 3s)$, and

$$\frac{1}{|\vec{r}-\vec{R}|} = \sum_{L=|l_1-l_2|}^{l_1+l_2} \frac{4\pi}{2L+1} \sum_{M=-L}^{L} Y_L^M(R) Y_L^{M^*}(r)[\frac{r^L}{R^{L+1}}\theta(R-r) + \frac{R^L}{r^{L+1}}\theta(r-R)] \tag{3.1}$$

We may write

$$\begin{aligned} I = & -\sum_{L=l_1-l_2}^{l_1+l_2} \frac{4\pi}{2L+1} \sum_{M=-L}^{L} \int r^{k_1+k_2} e^{-(\alpha_1+\alpha_2)r} \\ & * [\frac{r^L}{R^{L+1}}\theta(R-r) + \frac{R^L}{r^{L+1}}\theta(r-R)] r^2 dr \\ & * \int Y_{l_1}^{m_1^*} Y_{l_2}^{m_2} Y_L^M(R) Y_L^{M^*}(r) \sin\theta d\theta d\phi \end{aligned} \tag{3.2}$$

The radial part of this expression is

$$I_R = \int r^{k_1+k_2} e^{-(\alpha_1+\alpha_2)r} [\frac{r^L}{R^{L+1}}\theta(R-r) + \frac{R^L}{r^{L+1}}\theta(r-R)] r^2 dr \tag{3.3}$$

This is simplified considering

$$\int_0^\infty r^m e^{-\alpha r} dr = \frac{m!}{\alpha^{m+1}} \tag{3.4}$$

and

$$\int_0^R r^m e^{-\alpha r} = \frac{m!}{\alpha^{m+1}} - e^{-\alpha R} \sum_{b=0}^{m} \frac{m!}{b!} \frac{R^b}{\alpha^{m-b+1}} \tag{3.5}$$

to give

$$I_R = -\frac{(K+2+L)!}{\alpha^{K+3+L}} \frac{1}{R^{L+1}} + \frac{e^{-\alpha R}}{R^{L+1}} \sum_{b=0}^{K+2+L} \frac{(K+2+L)! R^b}{b! \alpha^{K+L+3-b}}$$
$$- e^{-\alpha R} \sum_{b=0}^{K+1-L} \frac{(K+1-L)!}{b!} \frac{R^{b+L}}{\alpha^{K+2-L-b}} \tag{3.6}$$

where $K = k_1 + k_2$ and $L = |l_1 - l_2| \sim |l_1 + l_2|$

(i) Excitation matrix elements for 1s-1s.

Taking the wave function for 1s as

$$\chi_{1s} = 2e^{-r} \sqrt{\frac{1}{4\pi}} e^{-iE_{1s}\frac{z}{v}} \tag{3.7}$$

and considering the fact that $l_1 = l_2 = L = M = 0$ and $K = 0$ we evaluate the excitation matrix element for 1s-1s using eq. (3.6) as

$$< \chi_{1s}| - \frac{1}{|\vec{r} - \vec{R}|} |\chi_{1s} >= \frac{-1}{R}[1 - e^{-2R}(1+R)] \tag{3.8}$$

(ii) Excitation matrix elements for $3s - 3s$.

The wave function for 3s is

$$\phi_{3s} = \sqrt{\frac{1}{4\pi}} (\frac{1}{3})^{\frac{3}{2}} [2 - \frac{4}{3}|\vec{r} - \vec{R}| + \frac{4}{27}|\vec{r} - \vec{R}|^2] e^{-\frac{|\vec{r}-\vec{R}|}{3}} e^{-iE_{3s}\frac{Z}{v}} e^{-i\frac{v}{2}Z} e^{i\vec{v}\cdot\vec{r}} \tag{3.9}$$

Taking $L = M = K = 0$ and using eq. (3.6), we have

$$< \phi_{3s}| - \frac{1}{r}|\phi_{3s} >= -\frac{1}{R}[1 - e^{-\frac{2}{3}R}(1 + \frac{5}{9}R + \frac{4}{27}R^2 + \frac{4}{81}R^3 - \frac{4}{27^2}R^4 + \frac{4}{27^2 \cdot 3}R^5)] \tag{3.10}$$

It can be shown that $< \chi_{3s}| - \frac{1}{|\vec{r}-\vec{R}|}|\chi_{3s} >$ gives the same result as in eq. (3.10). Eq. (3.6) may be used to calculate all excitation matrix elements for all $s-s$, $p-p$ and $s-p$ states.

CHAPTER FOUR

CHARGE TRANSFER MATRIX ELEMENTS

In this section we will discuss the calculations of the charge transfer matrix elements. A one-dimensional integral is derived to evaluate such matrix elements.

4.1 Evaluation of charge transfer matrix elements

In this method we use a Feynman integral technique to reduce the three dimensional integral into a one-dimensional integral. The basic integral used to evaluate the charge transfer matrix elements is

$$I_1 = \int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-i\vec{v}\cdot\vec{r}} \frac{e^{-\alpha r}}{r} d\vec{r} \tag{4.1}$$

where f and α are real constants related to the initial and final states. Introducing a Fourier transform $\frac{e^{-\alpha r}}{r}$, eq. (4.1) may be written as

$$I_1 = \int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{i(\vec{k}-\vec{v})\cdot(\vec{r}-\vec{R})} d\vec{r} \frac{1}{2\pi^2} \int_{-\infty}^{+\infty} \frac{e^{i(\vec{k}-\vec{v})\cdot\vec{R}}}{k^2+\alpha^2} d\vec{k} \tag{4.2}$$

After the r integral has been carried out, we find that

$$I_1 = \frac{2}{\pi} \int_{-\infty}^{+\infty} \frac{e^{i(\vec{k}-\vec{v})\cdot\vec{R}}}{(k^2+\alpha^2)(|\vec{k}-\vec{v}|^2+f^2)} d\vec{k} \tag{4.3}$$

Using Feynman identity

$$(ab)^{-1} = \int_0^1 \frac{dx}{[a+(b-a)x]^2} \tag{4.4}$$

Eq. (4.3) becomes

$$I_1 = \frac{2}{\pi} \int_0^1 dx \int_{-\infty}^{+\infty} \frac{e^{i(\vec{k}-\vec{v})\cdot\vec{R}}}{[(k^2+\alpha^2)+(|k-v|^2+f^2-k^2-\alpha^2)x]^2} d\vec{k}$$

$$= \frac{2}{\pi}\int_0^1 dx \int_{-\infty}^{+\infty} \frac{e^{i(\vec{P}+(x-1)\vec{v})\cdot\vec{R}}d\vec{p}}{[(\vec{P}+x\vec{v})^2+\alpha^2+(|\vec{P}+(x-1)\vec{v}|^2+f^2-(\vec{P}+x\vec{V})^2-\alpha^2)x]^2}$$

where $\vec{P} = \vec{k} - x\vec{v}$. Define $M = v^2x(1-x) + f^2 - \alpha^2 x + \alpha^2$. The denominator then reduces to

$$\begin{aligned}
&(\vec{P}+x\vec{v})^2+\alpha^2+(|\vec{P}+(x-1)\vec{v}|^2+f^2-(\vec{P}+x\vec{v})^2-\alpha^2)x \\
&= P^2 + v^2x(1-x) + (f^2-\alpha^2)x + \alpha^2 \\
&= P^2 + M
\end{aligned} \tag{4.5}$$

The remaining integral may be evaluated to finally give

$$I_1 = \int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} \frac{e^{-i\vec{v}\cdot\vec{r}}}{r} d\vec{r} = 2\pi \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}} \frac{e^{-\sqrt{M}R}}{\sqrt{M}} dx \tag{4.6}$$

To calculate charge transfer matrix elements, a differentiation with respect to $f, -\alpha$, or v has to be taken. Modified spherical Bessel function of the third kind h_n has been used to simplify the differentiation. The $H(n)$ functions are defined below to simplify the expressions of the formulas

$$H(n) = -i^n \frac{R^{2n+1}}{\rho^n} h_n(\rho_i) \tag{4.7}$$

where $\rho = \sqrt{M}R$

$$\frac{\partial H(n)}{\partial M} = \frac{\partial H(n)}{\partial \rho}\frac{\partial \rho}{\partial M} \tag{4.8}$$

But

$$\frac{\partial \rho}{\partial M} = \frac{R}{2\sqrt{M}} \tag{4.9}$$

and

$$\frac{\partial H(n)}{\partial \rho} = -i^n R^{2n+1} \frac{\partial(\frac{hn}{\rho^n})}{\partial \rho} = -i^n R^{2n+1} \cdot (-i) \frac{h_{n+1}}{\rho^n}(\rho_i) \tag{4.10}$$

From (4.7), (4.8) and (4.10)

$$\begin{aligned} \frac{\partial H(n)}{\partial M} &= \frac{R}{2\sqrt{M}}(-i^n) R^{2n+1} \cdot (-i) \frac{h_{n+1}}{\rho^n}(\rho_i) \\ &= \frac{i^{n+1}}{2} \frac{R^{2n+3}}{\rho^{n+1}} h_{n+1}(\rho_i) \end{aligned} \tag{4.11}$$

Also from (4.7)

$$H(n+1) = -i^{n+1} \frac{R^{2n+3}}{\rho^{n+1}} h_{n+1}(\rho_i) \tag{4.12}$$

Hence, comparing (4.11) and (4.12) we have

$$\frac{\partial H(n)}{\partial M} = -\frac{1}{2} H(n+1) \tag{4.13}$$

Using eq. (4.13) and defining $H(0)$ as $H(0) = \frac{e^{-\sqrt{M}R}}{\sqrt{M}}$, we obtain

$$H(0) = \frac{e^{-\sqrt{M}R}}{\sqrt{M}} = -Rh_0 \tag{4.14}$$

$$H(1) = \frac{e^{-\sqrt{M}R}}{M}(R + \frac{1}{\sqrt{M}}) = -\frac{R^3}{\rho} i h_1 \tag{4.15}$$

$$H(2) = \frac{e^{-\sqrt{M}R}}{M^{\frac{3}{2}}}(R^2 + \frac{3R}{\sqrt{M}} + \frac{3}{M}) = \frac{R^5}{\rho^2} h_2 \tag{4.16}$$

$$H(3) = \frac{e^{-\sqrt{M}R}}{M^{\frac{3}{2}}}(R^3 + \frac{6R^2}{\sqrt{M}} + \frac{15R}{M} + \frac{15}{M^{\frac{2}{3}}}) = \frac{R^7}{\rho^3} i h_3 \tag{4.17}$$

$$H(4) = \frac{e^{-\sqrt{M}R}}{M^{\frac{5}{2}}}(R^4 + \frac{10R^3}{\sqrt{M}} + \frac{45R^2}{M} + \frac{105R}{M^{\frac{3}{2}}} + \frac{105}{M^2}) = -\frac{R^9}{\rho^4} h_4 \tag{4.18}$$

The formulas which have been derived for the calculation of charge transfer elements for $s-s$, $s-p$ and $p-p$ in the proton-hydrogen scattering are given in appendix A. An example of such derivation is given below:

By differentiating eq. (4.6) with respect to $-\alpha$ we have

$$I_1 = \int_{-\infty}^{+\infty} \frac{e^{\prime\,|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} e^{-i\vec{v}\cdot\vec{r}} d\vec{r} = 2\pi\alpha \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}}(1-x)H(1)dx \qquad (4.19)$$

4.2 Calculation of charge transfers.

Considering the wave equations (2.20) and (2.21) for χ_{1s} and ϕ_{3s} , the charge transfer matrices were calculated as follows

$$< \chi_{1s}| - \frac{1}{r}|\phi_{3s} > = \int \sqrt{\frac{1}{4\pi}} 2e^{-r} e^{iE_{1s}\frac{z}{v}} (-\frac{1}{r})(\frac{1}{3})^{\frac{3}{2}} [2 - \frac{4}{3}|\vec{r}-\vec{R}| + \frac{4}{27}|\vec{r}-\vec{R}|^2]$$
$$* e^{\frac{-|\vec{r}-\vec{R}|}{3}} \sqrt{\frac{1}{4\pi}} e^{-iE_{3s}\frac{z}{v}} e^{-i\frac{v}{2}z} e^{i\vec{v}\cdot\vec{r}} d\vec{r} \qquad (4.21)$$

Taking

$$\rho = |\vec{r}-\vec{R}| \qquad (4.22)$$

we have

$$< \chi_{1s}| - \frac{1}{r}|\phi_{3s} >= \frac{1}{4\pi} e^{i(E_{1s}-E_{3s})\frac{z}{v}} e^{i\frac{v}{2}z} \cdot 2(\frac{1}{3})^{\frac{3}{2}} \int [2 - \frac{4\vec{\rho}}{3} + \frac{4}{27}\rho^2]$$

$$* e^{-\frac{1}{3}\vec{\rho}} (-\frac{1}{|\rho - R|}) e^{-i\vec{v}\cdot\vec{\rho}} e^{-|\vec{\rho}-\vec{R}|} d\vec{\rho} \qquad (4.23)$$

$$< \phi_{3s}| - \frac{1}{|\vec{r}-\vec{R}|}|\chi_{1s} > = \frac{1}{4\pi} e^{\frac{i(E_{3s}-E_{1s})z}{v}} e^{i\frac{v}{2}z} \cdot 2(\frac{1}{3})^{\frac{3}{2}} \int [2 - \frac{4}{3}|\vec{r}-\vec{R}|$$
$$+ \frac{4}{27}|\vec{r}-\vec{R}|^2] e^{-\frac{|\vec{r}-\vec{R}|}{3}} e^{-r} e^{-i\vec{v}\cdot\vec{r}} (-\frac{1}{|\vec{r}-\vec{R}|}) d\vec{r} \qquad (4.24)$$

$$< \chi_{1s}|\phi_{3s} >= \frac{1}{4\pi} e^{\frac{i(E_{1s}-E_{3s})Z}{v}} e^{i\frac{v}{2}z} \cdot 2(\frac{1}{3})^{\frac{3}{2}}$$
$$* \int e^{-\vec{\rho}} e^{-\frac{\rho}{3}} e^{-i\vec{v}\cdot\vec{r}} [2 - \frac{4}{3}\vec{\rho} + \frac{4}{27}\rho^2] d\vec{\rho} \qquad (4.25)$$

Using the integrals (A1)to (A7) (see appendix A), equations (4.23), (4.24) and (4.25) are evaluated.

4.3 Charge transfer cross sections.

The theoretical calculation of cross sections for the inelastic processes

$$H^+ + H(1s) \rightarrow H(3s) + H^+$$
$$\rightarrow H^+ + H(3s)$$

over a wide range of collision energies has been done by using the coupled channel-equation. Considering the equation

$$iv\frac{\partial \Psi}{\partial z} = H\Psi \qquad (4.26)$$

where

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r} - \frac{1}{|\vec{r} - \vec{R}|}$$

and

$$\Psi = a_{1s}\chi_{1s} + b_{3s}\phi_{3s} \qquad (4.27)$$

with

$$\chi_{1s} = \chi(\vec{r})e^{-iE_{1s}\frac{z}{v}} \qquad (4.28)$$

and

$$\phi_{3s} = \phi(|\vec{r} - \vec{R}|)e^{-iE_{3s}\frac{z}{v}}e^{-i\frac{v}{2}z}e^{i\vec{v}\cdot\vec{r}} \tag{4.29}$$

we have

$$iv\frac{\partial\chi_{1s}}{\partial z} = (-\frac{1}{2}\bigtriangledown^2 - \frac{1}{r})\chi_{1s}(\vec{r}) \tag{4.30}$$

and

$$iv\frac{\partial\phi_{3s}}{\partial z} = (-\frac{1}{2}\bigtriangledown^2 - \frac{1}{|\vec{r} - \vec{R}|})\phi_{3s} \tag{4.31}$$

Also from eq. (4.26) and eq. (4.27) we have

$$iv\frac{\partial a_{1s}}{\partial z} + iv\phi_{3s}\frac{\partial b_{3s}}{\partial z} = -a_{1s}\frac{1}{|\vec{r} - \vec{R}|}\chi_{1s} - b_{3s}\frac{1}{r}\phi_{3s} \tag{4.32}$$

Multiplying by $\int \chi_{1s}^* d\vec{r}$ and simplifying the result gives

$$iv\frac{\partial a_{1s}}{\partial z} = a_{1s} < \chi_{1s}| - \frac{1}{|\vec{r} - \vec{R}|}|\chi_{1s} > + b_{3s} < \chi_{1s}| - \frac{1}{r}|\phi_{3s} >$$

$$-iv < \chi_{1s}|\phi_{3s} > \frac{\partial b_{3s}}{\partial z} \tag{4.33}$$

Also multiplying eq. (4.32) by $\int \phi_{3s}^* d\vec{r}$ and simplifying gives

$$iv\frac{\partial b_{3s}}{\partial z} = a_{1s} < \phi_{3s}|\frac{1}{|\vec{r} - \vec{R}|}|\chi_{1s} > + b_{3s} < \phi_{3s}| - \frac{1}{r}|\phi_{3s} >$$

$$-iv < \phi_{3s}|\chi_{1s} > \frac{\partial a_{1s}}{\partial z} \tag{4.34}$$

It is deduced that as z approaches $-\infty$, $a_{1s}\rightarrow 1$ and $b_{3s}\rightarrow 0$. Using the probabilities for each B (see Fig. I) the cross section is calculated as

$$\sigma = 2\pi \int \rho_{ij} B \; dB = 2\pi \int |b_{3s}|^2 B dB$$

where ρ_{ij} is the probability for each B.

Cross sections for energies from 5-350 keV are computed (table I) and results plotted together with values obtained by Skakeshaft[33] and Rapp[32] (fig.II).

Table I. Charge transfer cross sections ($10^{-17} cm^2$)
for 1s-3s in proton-hydrogen scattering

Energy (keV)	Rapp	Shakeshaft	Present
5	-	-	0.009
6	0.11	-	0.019
9	0.03	-	0.055
10	-	-	0.074
12	0.13	-	0.134
15	-	0.53	0.265
16	0.09	-	0.313
20	0.12	-	0.485
25	0.18	0.93	0.611
30	-	-	0.643
40	0.36	0.67	0.558
50	-	0.45	0.425
60	-	0.29	0.309
70	0.12	-	0.223
75	-	0.14	0.189
100	0.01	-	0.086
200	-	-	0.007
300	-	0.003	0.001
350	-	-	0.0006

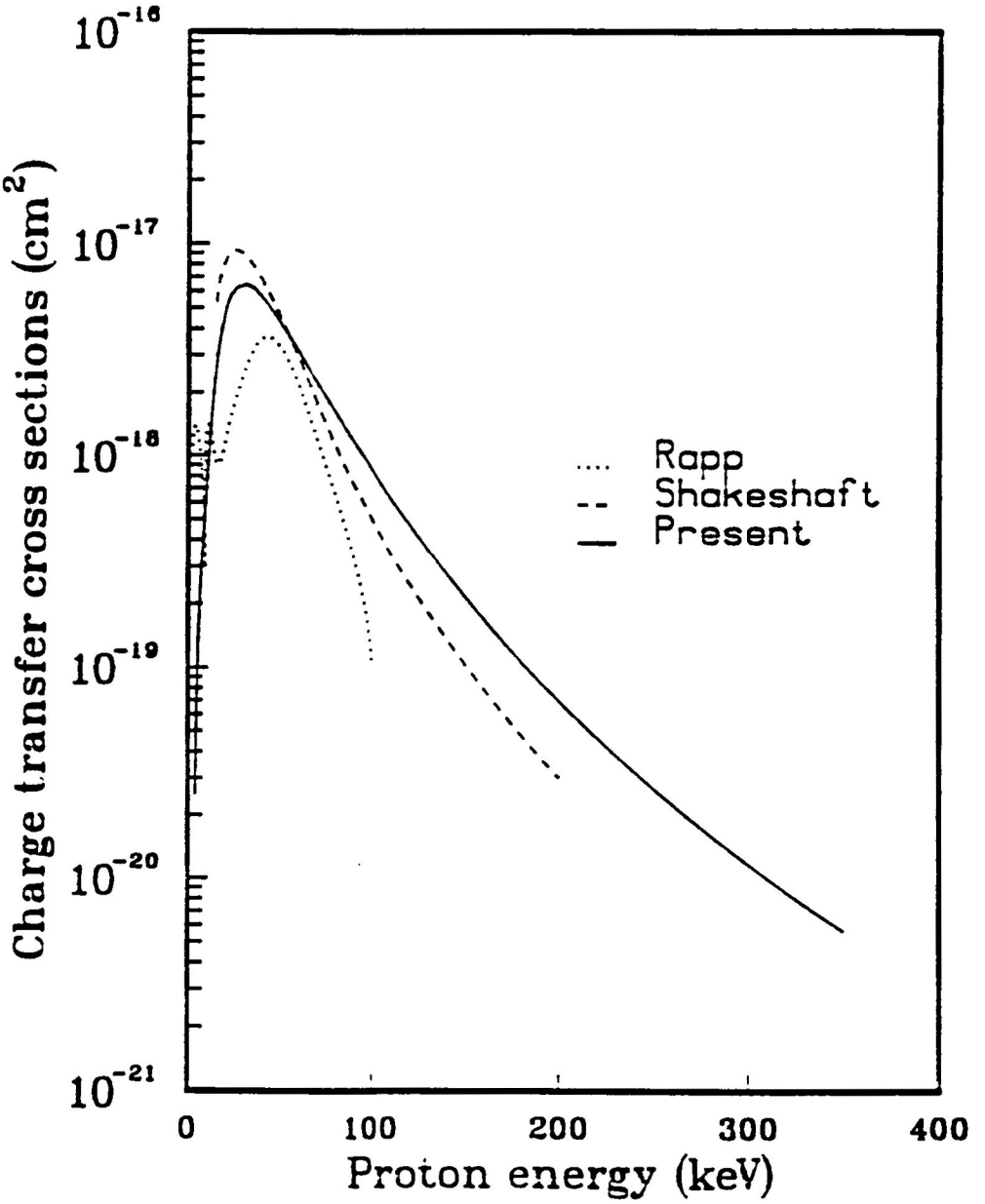

Fig II. Charge transfer cross sections for 1s-3s

CHAPTER FIVE
CONCLUSION

In this thesis a two-state coupled channel method has been used to calculate the charge transfer cross sections for hydrogen $1s$ to the $3s$ of the incoming proton.

The excitation matrix elements have been evaluated analytically. The charge transfer matrix elements are first reduced to one-dimensional integrals using a Feynman integral technique and then evaluated by using a Gauss-Lequerre quadrature method.

The two state coupled-channel equation is derived and used in the proton-hydrogen scattering. Charge transfer cross sections for hydrogen $1s$ to proton $3s$ have been computed in the energy range of 5-350 keV.

The curve in fig.II represents our data. The curve increases to a maximum at 30 keV and decreases very fast with increasing energy. Our results agree with those of Shakeshaft[33]. Rapp's [32] curve differs slightly and his peak is at around 40 keV.

We would like to extend this research to cover all $1s$ to $3p$ states on both target and projectile in future.

APPENDIX A

The formulas which are used to calculate charge transfer matrix elements are

$$\int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} \frac{e^{-i\vec{v}\cdot\vec{r}}}{r} d\vec{r} = 2\pi \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}} H(1) dx \tag{A1}$$

$$\int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} e^{-i\vec{v}\cdot\vec{r}} d\vec{r} = 2\pi\alpha \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}} (1-x) H(1) dx \tag{A2}$$

$$\int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} e^{-i\vec{v}\cdot\vec{r}} r d\vec{r} = 2\pi\alpha \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}} (1-x)[H(2)\alpha(1-x)$$

$$- \frac{H(1)}{\alpha}] dx \tag{A3}$$

$$\int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} e^{-i\vec{v}\cdot\vec{r}} r^2 d\vec{r} = 2\pi\alpha \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}} (1-x)^2 [H(3)*$$

$$* \alpha^2(1-x) - 3H(2)] dx \tag{A4}$$

$$\int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} e^{-i\vec{v}\cdot\vec{r}} |\vec{r}-\vec{R}| d\vec{r} = 2\pi\alpha f \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}} x(1-x)$$

$$H(2) dx \tag{A5}$$

$$\int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} e^{-i\vec{v}\cdot\vec{r}} |\vec{r}-\vec{R}|^2 d\vec{r} = 2\pi\alpha \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}} [f^2 x H(3)$$

$$- H(2)] x(1-x) dx \tag{A6}$$

$$\int_{-\infty}^{+\infty} \frac{e^{-f|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} e^{-\alpha r} e^{-i\vec{v}\cdot\vec{r}} |\vec{r}-\vec{R}|^3 d\vec{r} = 2\pi\alpha \int_0^1 e^{i(x-1)\vec{v}\cdot\vec{R}} [f^2 x H(4)$$

$$- 3H(3)] f x^2 (1-x) dx \tag{A7}$$

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